

BCS WORKSHOP

# **Calibration Strategies**

# 27<sup>th</sup> November 2009

KU Leuven Kasteelpark Arenberg 20 Auditorium Heuts B-3001 Heverlee

# Organisation:

# The Belgian Chemometrics Society

# http://chemometrie.kvcv.be

## Context

Multivariate calibration can be straightforward, if you have lots of clean data and future data will be like that. In practice, it is often more problematic, because these conditions are not met.

Chemometrics is more and more concerned with these problems. There are developments that aim at making models more robust, against strange samples in the calibration, against future disturbances, against the risks incurred when the calibration set is small.

Very many techniques and strategies have been proposed, and we haven't seen the end of it. So how do we go about a calibration problem in the presence of such a wealth of possibilities?

**Pierre Dardenne** presents strategies employed by contestants in the calibration shoot-out he organized for the French chemometrics conference Chimiométrie 2007.

Wouter Saeys gives an overview of techniques that aim at exploiting whatever knowledge is available on the system. E.g. if you have pure spectra available for potential impurities, this ought to help. **Sabine Verboven** will report on her work on applying a robust calibration scheme in order to protect against outliers in the data. This research was realized in cooperation with a Belgian animal feed company who provided real life NIR-spectra.

# Agenda

- 13.30 Welcome Coffee
- 14.00 Strategies in the Calibration shout-out of Chimiométrie 2007
   Pierre Dardenne, Quality of Agricultural Products department, CRA-W, Belgium
- 14.50 Exploiting additional information in calibration
  Wouter Saeys, Katholieke Universiteit
  Leuven, Department Biosystems
- 15.40 Coffee Break
- 16.00 Robust Calibration Sabine Verboven, Universiteit Antwerpen, Dept. of Mathematics, Statistics & Actuarial Science
- 16.50 Reception

#### Venue

The workshop will be hosted by KU Leuven, Department BIOSYST-MeBioS.

## Date of the workshop

November 27, 2009

## Fee

Participation to this workshop is €50, exclusive VAT.

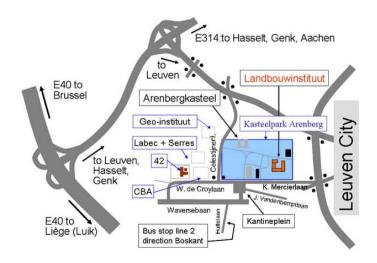
#### Registration

Registration is done by filling in the registration form at the website of the BCS (<u>http://chemometrie.kvcv.be/</u>).

### How to get to Kasteelpark Arenberg

For a detailed route description:

www.biw.kuleuven.be/English/routedescription.aspx



## Coming by car (to Kasteelpark Arenberg):

In the Celestijnenlaan go straight ahead, past the pedestrian crossing until the bridge over the river Dijle, after approximately 1 km. Take left and enter 'Kasteelpark Arenberg' immediately after the bridge. Follow the river Dijle, keeping the castle at your left and take the parking lot on your right-hand side. It is advised to leave your car here, because the rest of the park is only accessible for vehicles with a parking card. To go to Kasteelpark Arenberg 20 (Landbouwinstituut), continue following the river Dijle on foot until you see the main building of the Faculty on your right.

### By Train to Heverlee

At Leuven station you take the train to Wavre/Ottignies. Heverlee is the first stop. From Heverlee station it is a 10 minutes walk. Take the Sint-Lambertusstraat towards the church 'Sint-Lambertus'. Cross the 'Waversebaan', go straight on and follow 'Vandenbemptlaan' (turns to the left) till you reach a small square 'Kantineplein'.

Look for the castle and take the driveway to the castle (Kasteelpark Arenberg 1). To go to Kasteelpark Arenberg 20 (Landbouwinstituut) turn right at the castle. Follow the river Dijle until you see at your right, next to the road the main building of the Faculty.

#### The Belgian Chemometrics Society

The Belgian Chemometrics Society (BCS) operates as a section of the Royal Flemish Chemical Society (KVCV) and aims at promoting Chemometrics in Belgium with special attention for the interaction between academia and industry. Its main activity is the organisation of workshops and a bi-annual symposium.

Not a BCS member yet ? You are very welcome to join ! Just drop a line to chemometrie@kvcv.be

#### **BCS Committee members:**

Thomas De Beer Pierre Dardenne Bieke Dejaegher Juan Antonio Fernández Pierna Mauritz Kelchtermans Kristine Ooms Wouter Saeys Bas van den Bogaert